

\mathcal{PT} -Symmetric Quantum Theory Defined in a Krein Space

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Abstract

We provide a mathematical framework for \mathcal{PT} -symmetric quantum theory, which is applicable irrespective of whether a system is defined on \mathbb{R} or a complex contour, whether \mathcal{PT} symmetry is unbroken, and so on. The linear space in which \mathcal{PT} -symmetric quantum theory is naturally defined is a Krein space constructed by introducing an indefinite metric into a Hilbert space composed of square integrable complex functions in a complex contour. We show that in this Krein space every \mathcal{PT} -symmetric operator is \mathcal{P} -Hermitian if and only if it has transposition symmetry as well, from which the characteristic properties of the \mathcal{PT} -symmetric Hamiltonians found in the literature follow. Some possible ways to construct physical theories are discussed within the restriction to the class $\mathbf{K}(\mathbf{H})$.

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Since Bender and Boettcher claimed that the reality of the spectrum of the Hamiltonian $H = p^2 + x^2 + ix^3$ is due to the underlying \mathcal{PT} symmetry [1], there have appeared in the literature numerous investigations into various aspects of non-Hermitian Hamiltonians defined on, in general, a complex contour. By a simple argument, the eigenvalues of any \mathcal{PT} -symmetric linear operator are shown to be real unless the corresponding eigenvectors break \mathcal{PT} symmetry [2]. The examinations in the first four years (1998–2001) were mostly devoted to check this spectral property. For an extensive bibliography, see e.g. the references cited in Ref. [3]. Then Dorey *et al.* achieved the celebrated rigorous proof of a sufficient condition for the spectral reality of a multi-parameter family of a \mathcal{PT} -symmetric Hamiltonian [4].

Around the same period, the researchers in the field were gradually interested in the other important problems such as inner products, Hilbert spaces, completeness of the eigenvectors, and so on. These problems were already noticed and accessed in a couple of the earlier works [5, 6, 7], where a bilinear non-Hermitian form was introduced as a metric. Then the different groups arrived at the same sesquilinear Hermitian but indefinite form defined in the real line \mathbb{R} [8, 9], which was the origin of what has been sometimes called the \mathcal{PT} *inner product*. In particular, it was discussed in Ref. [8] that the state vector space with this indefinite metric is a Krein space and that the usual quantum mechanical description would be obtained for \mathcal{PT} -symmetric Hamiltonians as far as we ‘ignore’ the neutral eigenvectors. Some mathematical results of Krein space were also applied to a simple \mathcal{PT} -symmetric model defined in a finite real interval $[-1, 1] \subset \mathbb{R}$ in Ref. [10]. An apparent drawback of their metric is that it was defined only for wave functions of $L^2(\mathbb{R})$. Regarding the indefiniteness, Bender *et al.* in 2002 proposed a new operator \mathcal{C} , called *charge conjugation*, to construct a positive definite inner product for an unbroken \mathcal{PT} -symmetric model [11], expecting that a physically acceptable quantum theory would be obtainable with it. However, the \mathcal{C} operator depends on the Hamiltonian under consideration, and the explicit construction of the \mathcal{C} operator has been one of the current main issues, see e.g., [12, 13, 14].

On the other hand, Mostafazadeh employed the notion of *pseudo-Hermiticity* and tried to formulate \mathcal{PT} -symmetric theory within its framework [15]. For the development, see Ref. [16] and the references cited therein. However, the formulation has involved a defect from the beginning, since the (reference) Hilbert space is basically defined in \mathbb{R} and thus the formulation cannot be directly applied to the case where a \mathcal{PT} -symmetric operator is naturally defined on a complex contour. This problem was recently addressed for a couple of models in Ref. [17]. Besides this problem, we should call an attention to the more serious fact that until now little has been known about what kinds of (non-normal) pseudo-Hermitian operators in infinite-dimensional spaces certainly guarantee one of the key assumptions in the series of the papers, namely, the existence of a complete biorthonormal eigenbasis of the operators, as was questioned in Refs. [18, 19]. In this respect, we have presented a set of necessary conditions for the existence of biorthonormal eigenbasis of non-Hermitian operators in our previous paper [20]. Another important caution about pseudo-Hermiticity, namely, boundedness of metric operators, was recalled in Ref. [18]; see also Ref. [21].

In this letter, considering the present status in the field, we would like to propose a unified mathematical framework for \mathcal{PT} -symmetric quantum theory. Here by ‘unified’ we mean that its applicability does not rely on whether a theory is defined on \mathbb{R} or a complex contour, on whether \mathcal{PT} symmetry is unbroken, and so on. Furthermore, we clarify the relation between \mathcal{PT} symmetry and pseudo-Hermiticity in our framework. We then discuss some possibilities for constructing physical theories within our framework based on mathematically well-established results.

To begin with, let us introduce a complex-valued smooth function $\zeta(x)$ on the real line $\zeta : \mathbb{R} \rightarrow \mathbb{C}$ satisfying that (i) the real part of $\zeta(x)$ is monotone increasing in x and $\Re\zeta(x) \rightarrow \pm\infty$ as $x \rightarrow \pm\infty$, (ii) the first derivative is bounded, i.e., $(0 <) |\zeta'(x)| < C (< \infty)$ for all $x \in \mathbb{R}$, and (iii) $\zeta(-x) = -\zeta^*(x)$ where $*$ denotes complex conjugate. The function $\zeta(x)$ defines a complex contour in the complex plane and here we are interested in a family of the complex contours $\Gamma_a \equiv \{\zeta(x) | x \in (-a, a), a > 0\}$, which has mirror symmetry with respect to the imaginary axis. This family of complex contours would sufficiently cover all the support needed to define \mathcal{PT} -symmetric quantum mechanical systems. In particular, we note that Γ_∞ with $\zeta(x) = x$ is just the real line \mathbb{R} on which standard quantum mechanical systems are considered.

Next, we consider a complex vector space \mathfrak{F} of a certain class of complex functions and introduce a sesquilinear Hermitian form $Q_{\Gamma_a}(\cdot, \cdot) : \mathfrak{F} \times \mathfrak{F} \rightarrow \mathbb{C}$ on the space \mathfrak{F} , with a given $\zeta(x)$, by

$$Q_{\Gamma_a}(\phi, \psi) \equiv \int_{-a}^a dx \phi^*(\zeta(x)) \psi(\zeta(x)). \quad (1)$$

Apparently, it is positive definite, $Q_{\Gamma_a}(\phi, \phi) > 0$ unless $\phi = 0$, and thus defines an inner product on the space \mathfrak{F} . With this inner product we define a class of complex functions which satisfy $\lim_{a \rightarrow \infty} Q_{\Gamma_a}(\phi, \phi) < \infty$, that is, the class of complex functions which are square integrable (in the Lebesgue sense) in the complex contour Γ_∞ with respect to the *real* integral measure dx . We note that this class contains all the complex functions which are square integrable in Γ_∞ with respect to the complex measure dz along Γ_∞ thanks to the property (ii) of the function $\zeta(x)$. As in the case of $L^2(\mathbb{R})$, we can show that this class of complex functions also constitutes a Hilbert space equipped with the inner product $Q_{\Gamma_\infty}(\cdot, \cdot) \equiv \lim_{a \rightarrow \infty} Q_{\Gamma_a}(\cdot, \cdot)$, which is hereafter denoted by $L^2(\Gamma_\infty)$. A Hilbert space $L^2(\Gamma_a)$ for a finite positive a can be easily defined by imposing a proper boundary condition at $x = \pm a$.

Before entering into the main subject, we shall define another concept for later purposes. For a linear differential operator A acting on a linear function space of a variable x , $A = \sum_n \alpha_n(x) d^n/dx^n$, the transposition A^t of the operator A is defined by $A^t = \sum_n (-1)^n d^n/dx^n \alpha_n(x)$. An operator L is said to have *transposition symmetry* if $L^t = L$. If A acts in a Hilbert space $L^2(\Gamma_\infty)$, namely, $A : L^2(\Gamma_\infty) \rightarrow L^2(\Gamma_\infty)$, the following relation holds for all $\phi(z), \psi(z) \in \mathfrak{D}(A) \cap \mathfrak{D}(A^t) \subset L^2(\Gamma_\infty)$:

$$\lim_{a \rightarrow \infty} \int_{-a}^a dx \phi(\zeta(x)) A^t \psi(\zeta(x)) = \lim_{a \rightarrow \infty} \int_{-a}^a dx [A\phi(\zeta(x))] \psi(\zeta(x)). \quad (2)$$

With these preliminaries, we now introduce the linear parity operator \mathcal{P} which performs spatial reflection $x \rightarrow -x$ when it acts on a function of a real spatial variable x as $\mathcal{P}f(x) = f(-x)$. We then define another sesquilinear form $Q_{\Gamma_a}(\cdot, \cdot)_\mathcal{P} : \mathfrak{F} \times \mathfrak{F} \rightarrow \mathbb{C}$ by

$$Q_{\Gamma_a}(\phi, \psi)_\mathcal{P} \equiv Q_{\Gamma_a}(\mathcal{P}\phi, \psi). \quad (3)$$

We easily see that this new sesquilinear form is also Hermitian since

$$\begin{aligned} Q_{\Gamma_a}(\psi, \phi)_\mathcal{P} &= \int_{-a}^a dx \psi^*(-\zeta^*(x)) \phi(\zeta(x)) \\ &= \int_{-a}^a dx' \psi^*(\zeta(x')) \mathcal{P}\phi(\zeta(x')) = Q_{\Gamma_a}(\psi, \mathcal{P}\phi) \\ &= Q_{\Gamma_a}^*(\mathcal{P}\phi, \psi) = Q_{\Gamma_a}^*(\phi, \psi)_\mathcal{P}, \end{aligned} \quad (4)$$

where we use the Hermitian symmetry of the form (1) as well as the property (iii). However, it is evident that the form (3) is no longer positive definite in general. We call the indefinite sesquilinear Hermitian form (3) *\mathcal{P} -metric*.

We are now in a position to introduce the \mathcal{P} -metric into the Hilbert space $L^2(\Gamma_\infty)$. For all $\phi(z), \psi(z) \in L^2(\Gamma_\infty)$ it is given by $Q_{\Gamma_\infty}(\phi, \psi)_\mathcal{P} \equiv \lim_{a \rightarrow \infty} Q_{\Gamma_a}(\phi, \psi)_\mathcal{P}$. It should be noted that we cannot take the two limits of the integral bounds, $a \rightarrow \infty$ and $-a \rightarrow -\infty$, independently in order to maintain the Hermitian symmetry of the form given in Eq. (4). Hence, in contrast with Hilbert space of ordinary quantum mechanics, the integration in non-symmetrical region contradicts the very definition of the \mathcal{P} -metric. From the definition of \mathcal{P} and relation (4), we easily see that the linear operator \mathcal{P} satisfies $\mathcal{P}^{-1} = \mathcal{P}^\dagger = \mathcal{P}$, where \dagger denotes the adjoint with respect to the inner product $Q_{\Gamma_\infty}(\cdot, \cdot)$, and thus is a *canonical symmetry* in the Hilbert space $L^2(\Gamma_\infty)$ [22]. Hence, the \mathcal{P} -metric turns to belong to the class of J -metric and the Hilbert space $L^2(\Gamma_\infty)$ equipped with the \mathcal{P} -metric $Q_{\Gamma_\infty}(\cdot, \cdot)_\mathcal{P}$ is a Krein space, which is hereafter denoted by $L_\mathcal{P}^2(\Gamma_\infty)$. Similarly, a Hilbert space $L^2(\Gamma_a)$ with $Q_{\Gamma_a}(\cdot, \cdot)_\mathcal{P}$ is also a Krein space $L_\mathcal{P}^2(\Gamma_a)$.

Let us next consider a linear operator A acting in the Krein space $L_\mathcal{P}^2$, namely, $A : \mathfrak{D}(A) \subset L_\mathcal{P}^2 \rightarrow \mathfrak{R}(A) \subset L_\mathcal{P}^2$ with non-trivial $\mathfrak{D}(A)$ and $\mathfrak{R}(A)$. The \mathcal{P} -adjoint of the operator A is such an operator A^c that satisfies for all $\phi \in \mathfrak{D}(A)$

$$Q_{\Gamma_\infty}(\phi, A^c \psi)_\mathcal{P} = Q_{\Gamma_\infty}(A \phi, \psi)_\mathcal{P} \quad \psi \in \mathfrak{D}(A^c), \quad (5)$$

where the domain $\mathfrak{D}(A^c)$ of A^c is determined by the existence of $A^c \psi \in L_\mathcal{P}^2$. It is related to the adjoint operator A^\dagger in the corresponding Hilbert space L^2 by $A^c = \mathcal{P} A^\dagger \mathcal{P}$ with $\mathfrak{D}(A^c) = \mathfrak{D}(A^\dagger)$. A linear operator A is called *\mathcal{P} -Hermitian* if $A^c = A$ in $\mathfrak{D}(A) \subset L_\mathcal{P}^2$, and is called *\mathcal{P} -self-adjoint* if $\overline{\mathfrak{D}(A)} = L_\mathcal{P}^2$ and $A^c = A$ [22]. Here we note that the concept of *η -pseudo-Hermiticity* introduced in Ref. [15] is essentially equivalent to what the mathematicians have long called *G-Hermiticity* (with $G = \eta$) among the numerous related concepts in the field. Therefore, in this letter we exclusively employ the latter mathematicians' terminology to avoid confusion. Unless specifically stated, we follow the terminology after the book [22].

We now consider so-called \mathcal{PT} -symmetric operators in the Krein space $L_\mathcal{P}^2$. The action of the anti-linear time-reversal operator \mathcal{T} on a function of a real spatial variable x is defined by $\mathcal{T}f(x) = f^*(x)$, and thus $\mathcal{T}^2 = 1$ and $\mathcal{PT} = \mathcal{T}\mathcal{P}$ follow. Then an operator A acting on a linear function space \mathfrak{F} is said to be *\mathcal{PT} -symmetric* if it commutes with \mathcal{PT} , $[\mathcal{PT}, A] = \mathcal{PT}A - A\mathcal{PT} = 0$.

To investigate the property of \mathcal{PT} -symmetric operators in the Krein space $L_\mathcal{P}^2$, we first note that the \mathcal{P} -metric can be expressed as

$$Q_{\Gamma_a}(\phi, \psi)_\mathcal{P} = \int_{-a}^a dx [\mathcal{PT}\phi(\zeta(x))] \psi(\zeta(x)). \quad (6)$$

It is similar to but is slightly different from the (indefinite) \mathcal{PT} inner product in Ref. [11], and reduces to the one in Refs. [8, 9] if $\zeta(x) = x$ with $a \rightarrow \infty$.

Let A be a \mathcal{PT} -symmetric operator. By the definition (5), \mathcal{PT} symmetry, and Eqs. (2) and (6), the \mathcal{P} -adjoint of A reads

$$\begin{aligned} Q_{\Gamma_\infty}(\phi, A^c \psi)_\mathcal{P} &= \lim_{a \rightarrow \infty} \int_{-a}^a dx [\mathcal{PT}A\phi(\zeta(x))] \psi(\zeta(x)) \\ &= \lim_{a \rightarrow \infty} \int_{-a}^a dx [\mathcal{PT}\phi(\zeta(x))] A^t \psi(\zeta(x)) \\ &= Q_{\Gamma_\infty}(\phi, A^t \psi)_\mathcal{P}, \end{aligned} \quad (7)$$

that is, $A^c = A^t$ in $\mathfrak{D}(A^c)$ for an arbitrary \mathcal{PT} -symmetric operator A . Hence, a \mathcal{PT} -symmetric operator is \mathcal{P} -Hermitian in L_P^2 if and only if it has transposition symmetry as well. In particular, since every Schrödinger operator $H = -d^2/dx^2 + V(x)$ has transposition symmetry, \mathcal{PT} -symmetric Schrödinger operators are always \mathcal{P} -Hermitian in L_P^2 . The latter fact naturally explains the characteristic properties of the \mathcal{PT} -symmetric quantum systems found in the literature; indeed they are completely consistent with the well-established mathematical consequences of J -Hermitian (more precisely, J -self-adjoint) operators in a Krein space [22] with $J = \mathcal{P}$. Therefore, we can naturally consider any \mathcal{PT} -symmetric quantum system in the Krein space L_P^2 , regardless of whether the support Γ_∞ is \mathbb{R} or not, and of whether \mathcal{PT} symmetry is spontaneously broken or not. It should be noted, however, that the relation between \mathcal{PT} symmetry and J -Hermiticity (more generally G -Hermiticity) varies according to in what kind of Hilbert space we consider operators. This is due to the different characters of the two concepts; any kind of Hermiticity is defined in terms of a given inner product while \mathcal{PT} symmetry is not [19].

Before closing this letter, we shall discuss some possible ways to construct physical quantum theories defined in the Krein space L_P^2 . First of all, it would be to some extent restrictive to consider only operators with transposition symmetry although we are mostly interested in Schrödinger operators. For operators without transposition symmetry, \mathcal{PT} symmetry does not guarantee \mathcal{P} -Hermiticity. Hence, the requirement of \mathcal{PT} symmetry alone would be less restrictive as an alternative to the postulate of self-adjointness in ordinary quantum mechanics. Furthermore, there are several reasons that even the stronger condition of \mathcal{P} -self-adjointness would be unsatisfactory. In ordinary quantum mechanics, it is crucial that an arbitrary physical state can be expressed as a linear combination of eigenvectors of the Hamiltonian or physical observables under consideration. In this respect, it is important to recall the fact that this absolutely relies on the consequences of the self-adjointness, namely, the completeness of eigenvectors and the existence of an orthonormal basis composed of them. Unfortunately, however, J -self-adjoint operators generally guarantee neither of them; even the system of the root vectors of a J -self-adjoint operator does not generally span a dense set of the whole Krein space, and more strikingly, completeness of the system of the eigenvectors does not guarantee the existence of a basis composed of such vectors [22]. From this point of view, the so-called class $\mathbf{K}(\mathbf{H})$ [23] would be one of the most promising constraints in defining a physical theory.

A \mathcal{P} -self-adjoint operator A of the class $\mathbf{K}(\mathbf{H})$ is, roughly speaking, such an operator for which the Krein space L_P^2 admits a \mathcal{P} -orthogonal decomposition into invariant subspaces of A as

$$L_P^2 = [\dotplus]_{i=1}^\kappa [\mathfrak{S}_{\lambda_i}(A) \dotplus \mathfrak{S}_{\lambda_i^*}(A)] [\dotplus] L_P^{2'} \tag{8}$$

where $[\dotplus]$ denotes \mathcal{P} -orthogonal direct sum, κ is a *finite* number, $\lambda_i \notin \mathbb{R}$ are normal non-real eigenvalues of A , and $\mathfrak{S}_\lambda(A)$ is a subspace spanned by the root vectors corresponding to each eigenvalue λ :

$$\mathfrak{S}_\lambda(A) = \bigcup_{n=0}^{\infty} \text{Ker}((A - \lambda I)^n). \tag{9}$$

Relative to the above decomposition of the space, the operator A has a block diagonal form $A = \text{diag}(A_1, \dots, A_\kappa, A')$, where $A_i = A|_{\mathfrak{S}_{\lambda_i} \dotplus \mathfrak{S}_{\lambda_i^*}}$ and $A' = A|_{L_P^{2'}}$. The spectrum

of the operator A' is real, $\sigma(A') \subset \mathbb{R}$, and there is at most a *finite* number k of real eigenvalues μ_i for which the eigenspaces $\text{Ker}(A^{(\prime)} - \mu_i I)$ are degenerate. We note that all the subspaces $\mathfrak{S}_\lambda(A)$ corresponding to the non-real eigenvalues are *neutral*, that is, all the elements are \mathcal{P} -orthogonal to themselves. It is evident that when $\kappa = 0$, the operator A has no non-real eigenvalues. However, it does not immediately mean that \mathcal{PT} symmetry of the system is completely unbroken since eigenvectors belonging to real eigenvalues can break \mathcal{PT} symmetry. In this stronger sense, the class $\mathbf{K}(\mathbf{H})$ cannot characterize unbroken \mathcal{PT} symmetry perfectly, but it can certainly exclude a pathological case where an infinite number of neutral eigenvectors emerges. Now, a problem is how to deal or interpret the remaining finite number of neutral eigenvectors.

One possible way to construct a physical theory is to interpret the neutral eigenvectors belonging to non-real eigenvalues as physical states describing unstable decaying states (and their ‘spacetime-reversal’ states). After a sufficiently large time $t \rightarrow \infty$ (or $t \rightarrow -\infty$), the probability of observing these states would be zero. Thus in the *time-independent* description it indicates that they must have zero-norm for all $t \in (-\infty, \infty)$, which may be consistent with their neutrality. If such an interpretation turns to be indeed possible (though it is completely different from the traditional treatment such as optical potentials, complex coordinate rotations, and so on), \mathcal{P} -Hermitian quantum theory defined in the Krein space $L^2_{\mathcal{P}}$ would be able to describe, in particular, a system where stable bound states and unstable decaying states *coexist*, such as nuclear and hadron systems.

For the neutral eigenvectors corresponding to real eigenvalues, however, it seems difficult to make a reasonable physical interpretation. A simple way to avoid this difficulty is just to impose the additional condition $k = 0$. Another natural way of resolution is to consider the quotient space $\text{Ker}(A - \mu_i I) / \text{Ker}_0(A - \mu_i I)$ in each degenerate sector, where $\text{Ker}_0(A - \mu_i I)$ is the isotropic part of $\text{Ker}(A - \mu_i I)$. This prescription is somewhat reminiscent of the BRST quantization of non-Abelian gauge theories; the whole state vector space of the latter systems is also indefinite and the positive definite physical space is given by the quotient space $\text{Ker } \mathcal{Q}_B / \text{Im } \mathcal{Q}_B$, where \mathcal{Q}_B is a nilpotent BRST charge [24] and $\text{Im } \mathcal{Q}_B$ is the BRST-exact neutral subspace of the BRST-closed state vector space $\text{Ker } \mathcal{Q}_B$ [25] (for a review see, e.g., Ref. [26]). Under the condition $k = 0$ or the quotient-space prescription, the eigenvectors of A is complete in the Krein space $L^2_{\mathcal{P}}$ if and only if $\mathfrak{S}_\lambda(A) = \text{Ker}(A - \lambda I)$ for all eigenvalues λ (at least for bounded A) [27]. In this case, the system of eigenvectors can constitute an *almost* \mathcal{P} -orthonormalized basis of $L^2_{\mathcal{P}}$ [27], that is, it is the union of a finite subset of vectors $\{f_i\}_1^n$ and a \mathcal{P} -orthonormalized subset $\{e_i\}_1^\infty$ satisfying $Q_{\Gamma_\infty}(e_i, e_j)_{\mathcal{P}} = \delta_{ij}$ or $-\delta_{ij}$, these two subsets being \mathcal{P} -orthogonal to one another such that¹

$$L^2_{\mathcal{P}} = \overline{\langle f_1, \dots, f_n \rangle [\dot{+}] \langle e_1, e_2, \dots \rangle}. \quad (10)$$

As another possibility, we would like to mention about the \mathcal{CPT} inner product approach [11]. The linear charge-conjugation operator \mathcal{C} was originally introduced to obtain a positive definite inner product for the eigenvectors of \mathcal{PT} -symmetric operators when \mathcal{PT} symmetry is unbroken. In this sense, we do not need this kind of operator since we have already formulated the framework with a Hilbert space from the beginning, *irrespective of whether \mathcal{PT} symmetry is spontaneously broken or not*. Nevertheless, there could be another positive

¹ Precisely speaking, when we employ the quotient-space prescription, the Krein space in Eq. (10) should be read as $\hat{L}^2_{\mathcal{P}} = \mathfrak{L}_0^{[\perp]} / \mathfrak{L}_0$ where $\mathfrak{L}_0 = \langle \text{Ker}_0(A - \mu_i I) \mid i = 1, \dots, k \rangle$ is a neutral subspace of $L^2_{\mathcal{P}}$.

definite metric which is more suitable for our purpose. Suppose there is a *bounded*, \mathcal{PT} -symmetric linear operator \mathcal{C} with transposition symmetry in the Hilbert space L^2 (thus \mathcal{C} is \mathcal{P} -self-adjoint). Then a counterpart of \mathcal{CPT} inner product in our formulation would be the \mathcal{CP} -metric; indeed \mathcal{CP} is self-adjoint in L^2 and thus defines a metric, and we have

$$Q_{\Gamma_a}(\mathcal{CP}\phi, \psi) = \int_{-a}^a dx [\mathcal{CP}\mathcal{T}\phi(\zeta(x))] \psi(\zeta(x)). \quad (11)$$

Then, if \mathcal{C} is a \mathcal{P} -orthogonal projection such that $\mathcal{C} : L_{\mathcal{P}}^2 \rightarrow L_{\mathcal{P}}^{2'}$ and the \mathcal{CP} -metric is positive definite in $L_{\mathcal{P}}^{2'}$ (a trivial example is $\mathcal{C} = \text{diag}(0, \dots, 0, \mathcal{P}')$ relative to the decomposition (9), where $\mathcal{P}' = \mathcal{P}|_{L_{\mathcal{P}}^{2'}}$), the system would be essentially a \mathcal{P} -Hermitian operator A' defined in $L_{\mathcal{P}}^2$ now equipped with the positive definite \mathcal{CP} -metric. In contrast with the Hilbert space L^2 , the \mathcal{CP} -metric cannot be determined *a priori* since it depends on the structure of the decomposition (9) and the subspace $L_{\mathcal{P}}^{2'}$ for each given operator. Hence, it almost corresponds to the \mathcal{CPT} inner product in the case of unbroken \mathcal{PT} symmetry.

Finally, we should note that in several models investigated so far in the literature, there appears an infinite number of complex conjugate pair eigenvalues. In other words, the dimension of the neutral invariant subspace is infinite, and they do not belong to the class of $\mathbf{K}(\mathbf{H})$. Hence, such models would not be suitable for describing some physical systems, though their mathematical aspects are certainly interesting.

It should be also noted that the way to set up an eigenvalue problem for a given linear operator A is not unique. In this sense, our framework presented in this letter is just one possibility. Our premise is just the non-triviality of $\mathfrak{D}(A)$ and $\mathfrak{R}(A)$ in $L_{\mathcal{P}}^2$. On the other hand, the eigenvalue problems of \mathcal{PT} -symmetric polynomial-type potentials in the literature, such as Ref. [4], were usually set up within the framework of Ref. [28] without any metric. Hence, it is interesting to investigate the relation among the different setups of eigenvalue problems. For a recent study, see also Ref. [29].

A generalization of the framework to many-body systems (described by M spatial variables x_i) would be straightforward by introducing M complex-valued functions $\zeta_i(x_i)$ which satisfy similar properties of (i)–(iii) with respect to each variable x_i ($i = 1, \dots, M$).

Various physical consequences of \mathcal{PT} -symmetric theory in our framework would be reported in detail in a subsequent publication [30].

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